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Massless Parton Asymptotics within Variable Flavour Number Schemes

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Abstract

In this note we formulate and investigate theoretical uncertainties for high Q^2 deep inelastic heavy quark (charm, etc.) production rates which arise within collinear resummation techniques from variations of the *a priori* unknown charm input scale Q_0 of $\mathcal{O}(\alpha_s)$ variable flavour number schemes. We show that Q_0 variations constitute a source of considerable theoretical uncertainty of present $\mathcal{O}(\alpha_s)$ calculations within such schemes and we suggest to consider a scale optimization from higher order corrections. We also outline how the stability of the fixed order and collinearly resummed perturbation series for heavy quark production can be comparatively investigated by variation of Q_0.

The present discussion on the appropriate scheme for the perturbative treatment of the deep inelastic production of heavy quarks of mass $m \gg \Lambda_{QCD}$ can be partly traced back to the question what is the effective expansion parameter for high Q^2 predictions. While fixed order perturbation theory (FOPT) proceeds strictly stepwise in powers of $(\alpha_s/2\pi)$ at all scales, variable flavor number schemes (VFNSs) are based upon the expectation that terms $\sim (\alpha_s/2\pi \times \ln Q^2/m^2)^n$ from collinear regions in the phase space have to be resummed [1] to all perturbative orders n for high Q^2 when $(\alpha_s/2\pi \times \ln Q^2/m^2) \rightarrow \mathcal{O}(1)$. Such terms are undebatedly present in the high Q^2 limit of the perturbative partonic coefficient functions but their impact is less clear [2] on observable hadronic quantities like the charm component of the deep inelastic structure function F_2^c where the partonic coefficient functions have to be convoluted with modern, i.e. steep, parton distribution functions $\overset{(-)}{q}(x, \mu_F^2)$ and dominantly $g(x, \mu_F^2)$, $\mu_f \sim m$. The question which ordering of the perturbation series optimizes its convergence can therefore not be answered *a priori* but only from explicit quantitative, i.e. numerical investigations [2,3]; prominent tools for testing perturbative stability being K factor considerations [2] or scale variations [3]. At present both criteria indicate a well behaved fixed order perturbation series for relevant subasymptotic but large scales $Q \gg m$ [2–5]. As regards scale uncertainties, mainly variations of the mass factorization scale μ_F have been considered so far despite the fact that collinear resummation techniques introduce an additional arbitrary scale in the process set by the input scale Q_0 for the heavy quark:

Recently proposed variable flavour number schemes [6–10] for global PDF analyses are constructed upon the boundary condition

$$q_H^{(n_f+1)}(x, Q_0^2)\Big|_{Q_0=m} = 0 \tag{1}$$

for a heavy sea quark density to enter the massless partonic renormalization group (RG)-evolution equations which resum collinear splitting subdiagrams to all orders at the price of neglecting mass dependent terms. In Eq. (1) m is the heavy quark mass and the heavy quark input scale Q_0 is in more technical terms the transition (or *switching*) scale from a factorization scheme with n_f to the one with $n_f + 1$ partonic quark degrees of freedom

[11]. Since the scale Q_0 is of no physical meaning, a RG-like equation

$$\frac{\partial\, \mathcal{O}}{\partial \ln Q_0^2} = 0 \tag{2}$$

holds *ideally* for any heavy quark observable $\mathcal{O}$. At limited perturbative order, Eq. (2) will obviously be violated to some extent which we will investigate below for the charm contribution to the NC structure function $\mathcal{O} = F_2^c$.

At the heart of the variable flavour number schemes of [6–10] is some interpolation prescription between fixed order perturbation theory, assumed to be valid around $Q^2 = \mathcal{O}(m^2)$, and the $Q^2 \gg m^2$ massless parton (MP) asymptotics derived from the boundary condition in Eq. (1). To avoid within our rather general considerations a discussion of the peculiarities of the distinct heavy quark schemes we denote such interpolations very schematically as

$$\text{VFNS} = w(m^2/Q^2) \times \text{FOPT} + [1 - w(m^2/Q^2)] \times \text{MP}; \quad w \to \begin{cases} 1, \; m^2/Q^2 \to 1 \\ \\ 0, \; m^2/Q^2 \to 0 \end{cases} \tag{3}$$

where the simple weight w is meant to represent all the details of some elaborate scheme prescription [6–10, 12]. The deviation of VFNS from FOPT is thus *normalized* to MP and the predictive power of VFNS in Eq. (3) depends on the stability of the asymptotic MP prediction which is obtained from the boundary (1) at $Q_0 = m$ via massless RG evolutions. Equation (1) emerges from the matching conditions of a factorization scheme with n_f active flavours to a scheme with $n_f + 1$ active flavours at some *a priori* arbitrary transition (or *switching*) scale Q_0. The general transformation equations for quark (q) and gluon (g) parton densities as well as for α_s read up to NLO [11, 12]

$$
\begin{aligned}
q_H^{(n_f+1)}(x, Q_0^2) &= \frac{\alpha_s(Q_0^2)}{2\pi} \ln \frac{Q_0^2}{m^2} \int_x^1 \frac{d\xi}{\xi} P_{qg}^{(0)}(\xi)\, g^{(n_f)}\left(\frac{x}{\xi}, Q_0^2\right) &&+\; \mathcal{O}(\alpha_s^2) \\
g^{(n_f+1)}(x, Q_0^2) &= g^{(n_f)}(x, Q_0^2) \left(1 + \frac{\alpha_s(Q_0^2)}{6\pi} \ln \frac{m^2}{Q_0^2}\right) &&+\; \mathcal{O}(\alpha_s^2) \\
\alpha_s^{(n_f+1)}(Q_0^2) &= \alpha_s^{(n_f)}(Q_0^2) \Big/ \left(1 + \frac{\alpha_s(Q_0^2)}{6\pi} \ln \frac{m^2}{Q_0^2}\right) &&+\; \mathcal{O}(\alpha_s^3) \\
q^{(n_f+1)}(x, Q_0^2) &= q^{(n_f)}(x, Q_0^2) &&+\; \mathcal{O}(\alpha_s^2)
\end{aligned}
\tag{4}
$$

and obviously reduce to Eq. (1) for $Q_0 = m$:

$$q_H^{(n_f+1)}(x, m^2) = 0\;,\; g^{(n_f+1)}(x, m^2) = g^{(n_f)}(x, m^2)\;,\; \alpha_s^{(n_f+1)}(m^2) = \alpha_s^{(n_f)}(m^2)\;. \tag{5}$$

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In Eqs. (4) and (5) q_H introduces a partonic heavy quark density into the massless evolution equations and the unspecified $\alpha_s(Q_0^2)$ may be either $\alpha_s^{(n_f)}(Q_0^2)$ or $\alpha_s^{(n_f+1)}(Q_0^2)$ because the difference is of the orders neglected in (4). The argument of a continuous $g(x, Q_0^2)$ and $\alpha_s(Q_0^2)$ has been advanced [7, 11] for adopting $Q_0 = m$ in all NLO parton distribution sets constructed so far along a VFNS philosophy [13–15]. On the other hand, when $Q_0 \neq m$ the discontinuity of α_s is in practice as small as maximally 4% up to Q_0^2 as high as 1000 GeV^2. Anyway, the recently completed NNLO transformation equations [12, 16] reveal that the possibility of a continuous evolution across Q_0 breaks down beyond NLO by nonlogarithmic higher order corrections to (4), (5). The restriction to $Q_0 = m$ should hence be abandoned and effects of varying Q_0 should be taken into account on the same level as the variations of the mass factorization scale μ_F^2 usually considered. Indeed, along

$$\ln \frac{Q^2}{m^2} = \ln \frac{Q_0^2}{m^2} + \ln \frac{\mu_F^2}{Q_0^2} + \ln \frac{Q^2}{\mu_F^2} \qquad (6)$$

the two scales Q_0 and μ_F define quite symmetrically which portion of the quasi-collinear $\ln(Q^2/m^2)$ is actually resummed $[\ln(\mu_F^2/Q_0^2)]$ and what amount is kept at fixed order, either in the boundary condition for q_H $[\ln(Q_0^2/m^2)]$ or in the hard scattering coefficient function C_2^g in Eq. (7) below $[\ln(Q^2/\mu_F^2)]$. We will investigate the residual Q_0 dependence for the charm production contribution to the deep inelastic structure function F_2 using $m = m_c(= 1.5$ GeV$)$. To avoid complications from an interplay of several scales we will decouple the bottom and top quark from the process $(m_{b,t} \to \infty)$ and we will fix the factorization scale at $\mu_F = Q$.

In the asymptotic limit $m_c^2/Q^2 \to 0$ the schemes [7, 9, 10] reduce - as in Eq. (3) - to the so-called *Zero Mass Variable Flavour Number Scheme*, equivalent to the 'massless parton' scenario of Ref. [2] where any mass dependence is dropped except for the boundary conditions in (4). We will consider such a scenario in the following and ignore terms of $\mathcal{O}(m_c^2/Q^2)$ because these are not handled uniformly in the individual realizations [7, 9, 10] of a VFNS.[1] For definiteness we consider an $F_2^{c,MP}$ in $\gamma^* P$ scattering which is given by

$$\frac{1}{x} F_2^{c,MP}(x, Q^2) = e_c^2 \left\{ (c + \bar{c})(x, Q^2) + \frac{\alpha_s(Q^2)}{2\pi} \left[g \otimes C_2^g + (c + \bar{c}) \otimes C_2^q \right](x, Q^2) \right\} \quad , \quad (7)$$

[1]Indeed the charm scheme of [10] is explicitly constructed upon $Q_0 = m$ and a generalization of this particular scheme for $Q_0 \neq m$ seems nontrivial.
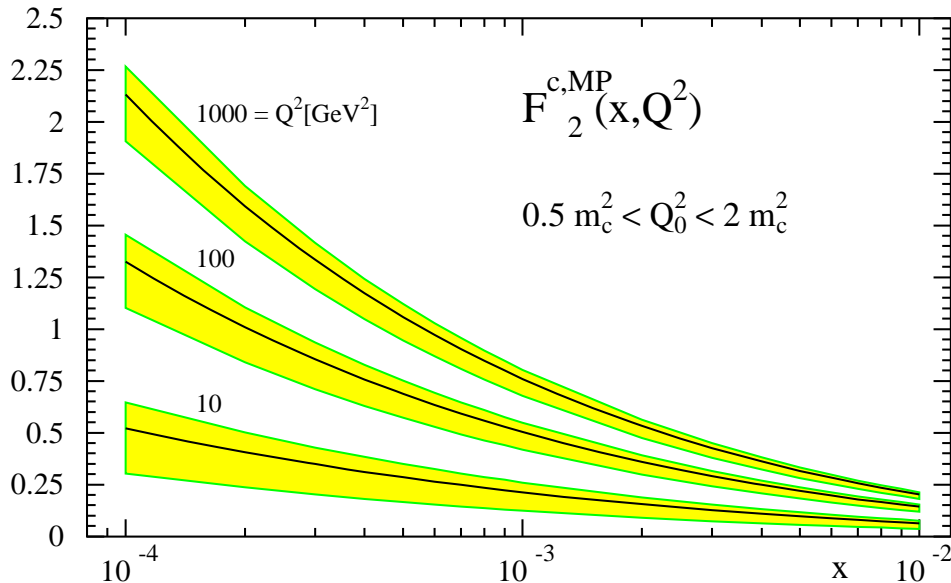
Figure 1: Dependence of the 'massless parton'-type charm structure function $F_2^{c,MP}$ in Eq. (7) on the switching scale Q_0 in the boundary conditions in Eq. (4). The solid lines represent the central value of $Q_0 = m_c$ and $F_2^{c,MP}$ decreases monotonically with increasing Q_0. The underlying parton distributions below Q_0 are those of Ref. [13].

where the $C_2^{g,q}$ are the massless $\overline{\rm MS}$ coefficient functions [17, 18]. It has already been pointed out in [2] that the 'massless parton' $F_2^{c,MP}$ in Eq. (7) can be rather arbitrarily suppressed if some larger *effective* charm mass is introduced [19] into the boundary condition (5). Our investigation here will clarify the situation if - for a fixed value of the *physical* charm mass m_c - the *unphysical* switching scale Q_0 is varied consistently according to the NLO boundary equations (4). Fig. 1 shows the effect if the transition scale is allowed to vary over the range $m_c^2/2 < Q_0^2 < 2\,m_c^2$ where the central value $Q_0 = m_c$ is represented by the solid lines and $F_2^{c,MP}$ monotonically decreases with increasing Q_0.[2] The evolution leading to the results in Fig. 1 is based on the $n_f = 3$ valence-like NLO input of Ref. [13] using NLO (2-loop) splitting functions. Above Q_0 the evolution deviates from [13] because we consider general $Q_0 \neq m_c$ here and we ignore - as mentioned above - any bottom quark effects ($m_b \to \infty$). The amount of change of $F_2^{c,MP}$ under variation of Q_0 hints at a reasonable perturbative stability. Nevertheless, the error represented by the

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[2] Allowing for $Q_0 < m_c$ in Eq. (4) leads obviously to $c(x, Q_0^2) < 0$ which appears somewhat counter-intuitive in probabilistic parton model language. Note, however, that a negative charm input arises even for $Q_0 = m$ from higher order corrections to Eq. (4) [20]. Anyway, the *measurable* cross section F_2^c is certainly positive above the physical threshold $Q^2(1/x - 1) > 4m_c^2$.
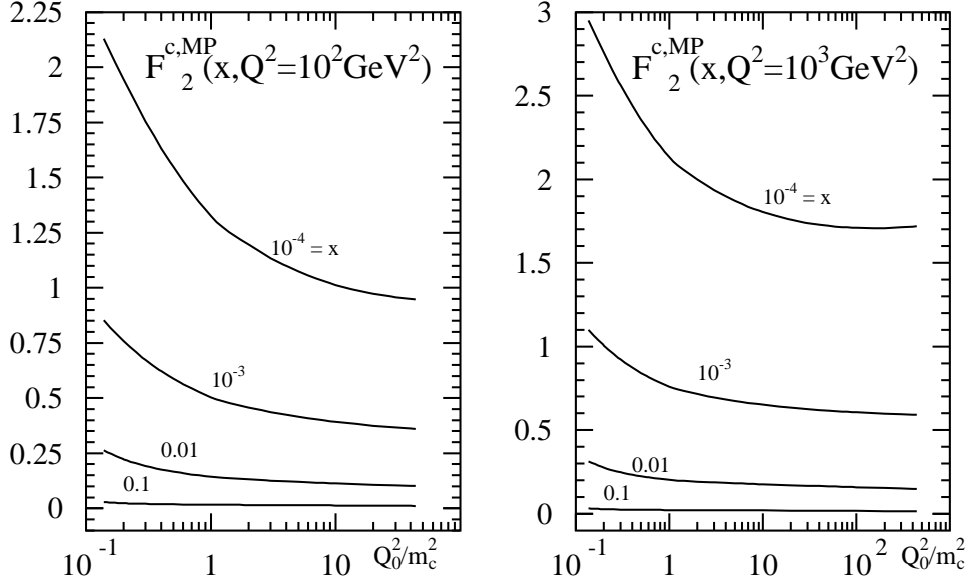
Figure 2: Dependence of the 'massless parton'-type charm structure function $F_2^{c,MP}$ in Eq. (7) on the switching scale Q_0 in the boundary conditions in Eq. (4). In this Figure Q_0 is allowed to vary (maximally) between the input scale of [13] as a lower and the physical scale Q^2 as an upper limit.

shaded bands in Fig. 1 is of the typical order of discrepancies between VFNS and FOPT calculations [10, 12] which questions the gain in predictivity if FOPT is abandoned for VFNS. Such uncertainties are critical for precise charm predictions to compare with future experimental accuracy, especially at experimentally most relevant intermediate scales and regarding the fact that Q_0^2 was only allowed to fluctuate by a factor of 2. This latter limitation rests on the assumption that Q_0 has to be very close to m_c for the all-order logarithms $(\alpha_s/2\pi \times \ln Q^2/m_c^2)^n$ to be correctly resummed. One can as well adopt a very different point of view towards the choice of Q_0. One can easily see that inserting Eq. (4) into Eq. (7) gives

$$\lim_{Q_0 \to Q} F_2^{c,MP}(x, Q^2) = \left[F_2^{GF} \otimes \left(1 + \frac{\alpha_s}{2\pi} C_2^q \right) \right] (x, Q^2) + \mathcal{O}\left(\alpha_s^2 \right) + \mathcal{O}\left(\frac{m_c^2}{Q^2} \right) \quad (8)$$

which is dominated by the $\mathcal{O}[\alpha_s \ln(Q^2/m_c^2)]$ LO gluon fusion term F_2^{GF} of the fixed order perturbation series. We may hence consider $Q_0 \to Q$ in a sense as a continuous path from variable flavour number to fixed order calculations. We should then consider values of Q_0 as high as we trust fixed order perturbation theory. In Fig. 2 we cover the maximally conceivable range for Q_0^2; i.e. the leftmost end of all curves is set by the low input scale of the parton distributions in [13], $Q_0^2 = 0.3$ GeV^2, while the rightmost ends are the 'fixed

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order limit' in Eq. (8). The observed monotonic scale dependence has to be expected from the positivity of the collinear resummation at small x which is continuously suppressed the more Q_0 is increased. Worrisome is, however, the steep slope $\partial F_2^{c,MP}/\partial \ln(Q_0^2/m_c^2)$ around $Q_0 \sim m_c$ for high $W^2 = Q^2(1/x - 1)$, where the charm contribution is most important. This observation restricts the predictive power of NLO collinear resummation techniques which have thus far been constructed to match the asymptotic $(Q^2 \to \infty)$ $F_2^{c,MP}$ derived from $c(x, Q_0^2 = m_c^2) = 0$. The uncertainty from the residual Q_0 dependence, inherent to any VFNS [7, 9, 10] worked out to NLO, seems to dominate over scheme uncertainties of $\mathcal{O}(m_c^2/Q^2)$ between the individual schemes. The arbitrariness of Q_0 therefore constitutes a main limiting factor on the perturbative accuracy of VFNS heavy quark predictions at high Q^2. On the other hand we observe a flattening slope $\partial F_2^{c,MP}/\partial \ln(Q_0^2/m_c^2)$ towards the 'fixed order limit' at high $Q_0 \lesssim Q$ where perturbative NLO $\leftrightarrow$ LO stability had been found in [2] by K factor considerations for the *full* fixed order predictions, i.e. including logs *and* finite terms. We should reemphasize that these conclusions are based on the NLO matching conditions in Eq. (4) - which is the present state of the art for PDF sets including partonic heavy quarks [13–15] - and do not take into account the higher corrections of [12, 16]. The terms beyond Eq. (4) represent NNLO contributions to the asymptotic VFNS prediction $F_2^{c,MP}$. Very recently the results of [12] have been implemented in a $\mathcal{O}(\alpha_s^2)$ implementation of a VFNS[3] where the contribution from the unknown NNLO (3-loop) splitting functions had to be neglected. Choosing $Q_0 = m$ the results of [20] seem to indicate that the impact of terms from the resummation beyond fixed NLO $[\mathcal{O}(\alpha_s^2)]$[4] perturbation theory is rather moderate. As a further step in the line of the present investigation it would clearly be interesting to generalize [20] to $Q_0 \neq m$. If a $Q_0 > m$ would be prefered by such an analysis the difference between VFNS and FOPT would be reduced even more. Such a result would again re-confirm the perturbative reliability of FOPT found in [2] as much as it would help reduce unphysical scheme dependences of QCD predictions on charm production and thus make a comparison to experiment even

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[3]A $c(x, Q^2)$ derived from the NNLO boundary conditions in [12] would, however, be problematic to apply to hadroproduction calculations, since the higher terms in [12] are not yet contained in, e.g., the fixed NLO $[\mathcal{O}(\alpha_s^3)]$ hadroproduction process $p\bar{p} \to c(p_T)X$ [21].

[4]The confusion of counting perturbative orders differently in resummed (MP) and fixed order (FOPT) calculations is treated in more detail in [8, 10].

more compelling.

To summarize, we have considered variations of the *a priori* arbitrary charm input scale Q_0, which separates a 3 from a 4 flavour scheme in variable flavour number approaches, around its usually adopted but by no means theoretically required value of $Q_0 = m_c$. From the NLO boundary conditions we found a monotonic Q_0 dependence and a worrisome steep slope of $F_2^{c,MP}$ in (7) with respect to $\ln Q_0^2$ just around $Q_0 \sim m_c$. This behaviour restricts the accuracy of a collinearly resummed NLO approach towards calculating high Q^2 charm production from matching $\mathcal{O}(\alpha_s)$ boson gluon fusion at $Q_0 = m_c$ in the MP component of Eq. (3). This uncertainty in MP from the unknown Q_0 feeds back onto the entire VFNS via Eq. (3) which is normalized to MP asymptotically ($Q^2 \gg m^2$). Our results imply to consider variations of Q_0 both as a limiting factor on the present perturbative accuracy if estimating the theoretical uncertainty of VFNS heavy quark predictions as well as in order to optimize the starting scale for the charm evolution within higher order realizations of VFNSs [12, 20, 22]. This latter higher order analysis assumes, however, that the unknown NNLO (3-loop) splitting functions can be neglected [20].

Acknowledgements

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